

Hypergraph states in Grover's quantum search algorithm

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Abstract. We study the entanglement content of the states employed in the Grover algorithm after the first oracle call when a few searched items are concerned. We then construct a link between these initial states and hypergraphs, which provides an illustration of their entanglement properties.

1. Introduction

Even though entanglement is considered as a major resource in quantum information processing, the role it plays in achieving the quantum computational speed-up in the currently known quantum algorithms still remains to be elucidated. In Ref. [1] it was shown that in Shor's algorithm multipartite quantum entanglement is needed to attain exponential computational speed-up. The presence of multipartite entanglement in the Deutsch-Jozsa algorithm and in the initial step of the Grover algorithm was pointed out recently [2]. Moreover, multipartite entanglement was shown to be present at each computational step in Grover's algorithm and a scale invariance property of entanglement dynamics was proved [3]. Lately, the notion of quantum hypergraph states was put forward and their link to states employed in the Deutsch-Jozsa and Grover algorithms was proved [4]. In this paper we consider the initial states employed in the Grover algorithm for a small number of searched solutions, study their entanglement content (in terms of the geometric measure of entanglement) and show the explicit connection to hypergraph states.

The paper is organised as follows. In Sect. 2 we review the notion of multi-qubit real equally weighted states and their link to hypergraphs. In Sect. 3 we consider the Grover algorithm and analyse the entanglement content of the corresponding states in the initial step of the algorithm for different numbers of solutions. We derive the hypergraphs underlying these symmetric initial states for one and two solutions in Sect. 4, and we finally summarise the main results in Sect. 5.

2. Real equally weighted states and hypergraphs

The n -qubit register employed in the Deutsch-Jozsa [5] and in the Grover [6] algorithms is initially prepared in state

$$|\psi_0\rangle \equiv \frac{1}{\sqrt{2^n}} \sum_{x=0}^{2^n-1} |x\rangle, \quad (1)$$

which corresponds to the equally weighted superposition of all possible 2^n states $|x\rangle$ in the computational basis. The next step in both algorithms consists in applying a unitary transformation U_f which generates the state

$$|\psi_f\rangle \equiv \frac{1}{\sqrt{2^n}} \sum_{x=0}^{2^n-1} (-1)^{f(x)} |x\rangle, \quad (2)$$

where $f(x)$ is the $\{0,1\}^n \rightarrow \{0,1\}$ Boolean function that needs to be evaluated in the considered algorithm. Notice that $(-1)^{f(x)} = \pm 1$ is just a real phase factor. The above states are referred to as multi-qubit “real equally weighted states” (REW) $|\psi_f\rangle$.

The REW states were recently linked to hypergraphs and the set of REW states was proved to be the same as the one of quantum hypergraph states [4]. A quantum hypergraph state is defined as follows. A hypergraph $g_{\leq n} = \{V, E\}$ is a set of n vertices V with a set of hyperedges E of any order k ranging from 1 to n (a hyperedge of order k connects a set of k vertices). Given a mathematical hypergraph, the corresponding quantum state can be found by following the three steps: assign to each vertex a qubit and initialise each qubit as $|+\rangle$ (the total initial state is then denoted by $|\psi_0\rangle$). Wherever there is a hyperedge, perform a controlled- Z operation between all connected qubits. Formally, if the qubits i_1, i_2, \dots, i_k are connected by a k -hyperedge, then perform the operation $C^k Z_{i_1 i_2 \dots i_k}$. The gate $C^k Z_{i_1 i_2 \dots i_k}$ introduces a minus sign to the input state $|11\dots 1\rangle_{i_1 i_2 \dots i_k}$, i.e. $C^k Z_{i_1 i_2 \dots i_k} |11\dots 1\rangle_{i_1 i_2 \dots i_k} = -|11\dots 1\rangle_{i_1 i_2 \dots i_k}$, and leaves all the other components of the computational basis unchanged. In this way we get the quantum state

$$|g_{\leq n}\rangle = \prod_{k=1}^n \prod_{\{i_1, i_2, \dots, i_k\} \in E} C^k Z_{i_1 i_2 \dots i_k} |\psi_0\rangle, \quad (3)$$

where $\{i_1, i_2, \dots, i_k\} \in E$ means that the k vertices are connected by a k -hyperedge. Notice that the product concerning the index $k = 1, 2, \dots, n$ accounts for different types of hyperedges in the hypergraph. We remind the reader that the well known graph states constitute a subset of quantum hypergraph states: they correspond to ordinary graphs, namely hypergraphs with all hyperedges being of order $k = 2$. In the following sections we will discuss some explicit examples of hypergraph states that appear in Grover's algorithm.

3. Initial states in Grover's algorithm

In this section we focus on the case of Grover's algorithm. The state (2) is achieved after the first application of the oracle. In this case the function f has output 1 for

entries x that correspond to solutions of the search problem and output 0 for values of x that are not solutions. We denote with M the number of solutions, which typically is much smaller than the total number of entries 2^n .

We will now study the entanglement properties of states (2) as functions of the number of qubits n for a fixed small number of solutions, i.e. $M = 1, 2$. We will quantify the amount of entanglement by the geometric measure of entanglement [7], which for a pure n -partite state $|\psi\rangle$ reads

$$E_q(|\psi\rangle) = 1 - \max_{|\phi\rangle \in S_q} |\langle\psi|\phi\rangle|^2, \quad (4)$$

where S_q represents the set of q -separable states, i.e. states that are separable with respect to q partitions. Notice that E_n quantifies the amount of entanglement of any kind contained in the global system, i.e. it is non-vanishing even for states showing entanglement just between two subsystems, while E_2 quantifies genuine multipartite entanglement. In the paper we will compute E_n .

We first review the case of a single solution to the search problem ($M = 1$), considered in [2]. Without loss of generality, as will be proved later, we consider the state representing the solution to be invariant under any permutation of the n qubits (e.g. $|111\dots 1\rangle$). Therefore, the state $|\psi_{M=1}\rangle$ after the oracle call, is also permutation invariant. We first compute E_n for this set of states, as a function of the number of qubits n . Due to the symmetry property, the search for the maximum in Eq. (4) can be restricted to symmetric separable states $|\phi\rangle^{\otimes n}$ [8], so that the maximisation involves only the two parameters $\alpha \in [0, \pi]$ and $\beta \in [0, 2\pi]$ that define the single qubit state $|\phi\rangle = \cos \frac{\alpha}{2} |0\rangle + e^{i\beta} \sin \frac{\alpha}{2} |1\rangle$.

The geometric measure of entanglement E_n for $M = 1$, i.e. for one solution of the search algorithm, thus reads

$$E_n(|\psi_{M=1}\rangle) = 1 - \max_{\alpha, \beta} \frac{1}{2^n} \left| \left(\cos \frac{\alpha}{2} + e^{i\beta} \sin \frac{\alpha}{2} \right)^n - 2e^{i\beta} \sin \frac{\alpha}{2} \right|^2. \quad (5)$$

The optimal value of β can be shown to be zero by induction over the number n of qubits, while the optimal α can be determined by explicitly calculating the derivative of the overlap, and then finding the root of a polynomial in $t = \tan \frac{\alpha}{2}$.

In Fig. 1 (Left) we show the behaviour of $E_n(|\psi_{M=1}\rangle)$, as a function of the number of qubits n . As we can see, the amount of entanglement decreases for increasing number of qubits. Notice however that, as shown in [3], even though the state shows an infinitely small amount of entanglement, it is genuine multipartite entangled.

We point out that the above results which were explicitly derived for permutation invariant states hold also for any Grover search with one searched item. Actually, all these states can be achieved from a symmetric state by applying tensor products of σ_x Pauli operators and identity operators $\mathbf{1}$ (e.g. $|001\dots 1\rangle = \sigma_{x1} \otimes \sigma_{x2} \otimes \mathbf{1}_3 \dots |111\dots 1\rangle$). Since these operations are local, they do not change the entanglement content of the resulting state.

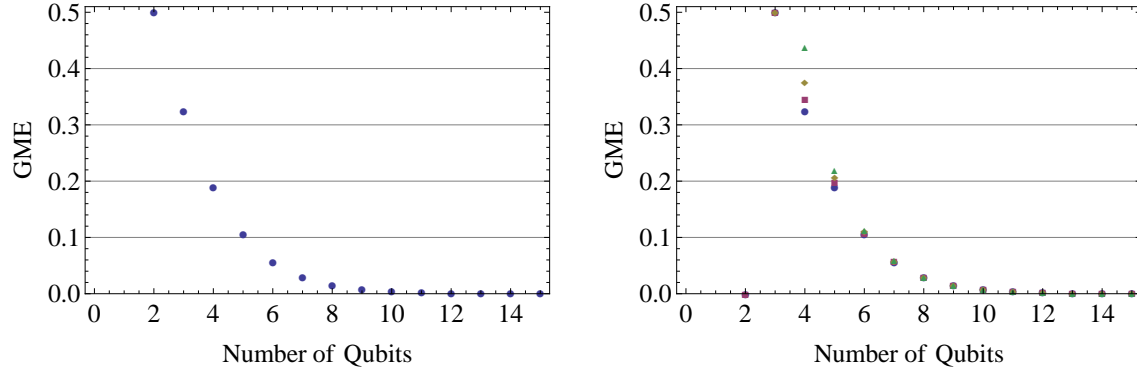


Figure 1. Left: Geometric measure of entanglement $E_n(|\psi_{M=1}\rangle)$ as a function of the number of qubits n for a single searched item. Right: $E_n(|\psi_{M=2}\rangle)$ as a function of the number of qubits n for two searched items; several values of the Hamming distance d are considered: $d = 1$ blue dots, $d = 2$ purple squares, $d = 3$ yellow diamonds, $d = 4$ green triangles.

We now focus on the states employed in the case of two solutions of the search problem ($M = 2$), i.e. states (2) with two minus signs. We introduce a classification of these states based on the Hamming distance d between the two computational basis states representing the solutions. We will show that the entanglement properties of the regarded states depend crucially on the number of digits in which the two solutions differ, i.e. on their Hamming distance d .

Without loss of generality, as will be proved below, we consider first the case in which the two n -qubit states representing the solutions differ in the first d digits and are invariant under permutations of the first d and last $n - d$ qubits, respectively (e.g. $|\underbrace{0\dots 0}_d \underbrace{1\dots 1}_d\rangle$ and $|\underbrace{1\dots 1}_d \underbrace{1\dots 1}_{n-d}\rangle$). We first compute E_n for this set of states, as a function of n . Due to the permutation invariance property, the search for the closest separable state, appearing in the geometric measure of entanglement, can still be restricted to separable states that show the same symmetry [8], i.e. $|\phi\rangle^{\otimes d}|\varphi\rangle^{\otimes n-d}$. Therefore the maximisation involves only the four parameters $\alpha, \gamma \in [0, \pi]$ and $\beta, \delta \in [0, 2\pi]$ that define the two single qubit states $|\phi\rangle$ and $|\varphi\rangle$.

The geometric measure of entanglement E_n for two solutions with Hamming distance d then takes the form

$$E_n(|\psi_{M=2}\rangle) = 1 - \max_{\alpha, \beta, \gamma, \delta} \frac{1}{2^n} \left| \left(\cos \frac{\alpha}{2} + e^{i\beta} \sin \frac{\alpha}{2} \right)^d \left(\cos \frac{\gamma}{2} + e^{i\delta} \sin \frac{\gamma}{2} \right)^{n-d} - 2e^{i(n-d)\delta} \sin^{n-d} \frac{\gamma}{2} \left(\cos^d \frac{\alpha}{2} + e^{id\beta} \sin^d \frac{\alpha}{2} \right) \right|^2. \quad (6)$$

Notice that when $d = n$ the maximisation procedure involves only two parameters: In this case the state is completely invariant under any permutation of the qubits, and thus only two parameters are needed.

As before, the optimal parameters α, β, γ and δ can be computed by maximising the squared overlap numerically. The corresponding results are reported in Fig. 1 (Right),

where the geometric measure of entanglement is plotted versus the number of qubits n . Notice that the state of two qubits is always separable for $M = 2$ and that $E_n(|\psi_{M=2}\rangle)$ for three qubits collapses to the single value $1/2$. As in the case $M = 1$, we can see that E_n approaches zero exponentially fast for increasing n . This behaviour holds for any finite value of the Hamming distance d . Notice also that for fixed finite number of qubits n the Hamming distance plays a crucial role for the amount of entanglement, since states with two solutions with higher distance d exhibit a higher amount of entanglement.

Finally, notice that all the results presented so far, even if they were explicitly derived for partially permutation invariant states, hold for any Grover search algorithm with two searched items. Actually, analogously to the case of a single solution discussed above, also for $M = 2$ all these states with fixed Hamming distance d can be reached from a partially symmetric one by applying tensor products of σ_x Pauli operators and identity operators $\mathbf{1}$ and/or permutations of the n qubits. As for the single solution case, since these operations are local, they do not change the entanglement content of the resulting state.

As mentioned in Sect. 2 all the above states are REW states and therefore they correspond to hypergraphs. In the next section we show how to relate states with $M = 1, 2$ to hypergraphs.

4. Connection to hypergraph states

Quantum hypergraph states, as reviewed in Sect. 2, allow us to describe the initial states employed in the Grover algorithm in a very convenient way. Indeed, entanglement properties and the gates (of the CZ type) that we explicitly need in order to generate them from the separable state $|\psi_0\rangle$ emerge very naturally from their hypergraph structure.

Consider first the initial symmetric state $|\psi_{M=1}\rangle$ (with a minus sign in front of the component $|111\dots 1\rangle$). It is straightforward to see that it corresponds to the hypergraph with the unique hyperedge of order n . Therefore, it has a very simple structure in the light of hypergraphs, showing clearly the presence of multipartite entanglement.

In order to discuss the case with two minus signs, we first notice that the hyperedge of order n will never appear now. Hence, even though states $|\psi_{M=2}\rangle$ might have a much more complicated hypergraph structure than $|\psi_{M=1}\rangle$, the gate $C^n Z$ will never be involved. This is because the state $|\psi_{M=2}\rangle$ has an even number of minuses, while any product of $C^k Z$ operators involving the gate $C^n Z$ is diagonal in the computational basis with an odd number of minus signs. We now discuss the general rule to find the hypergraph associated to the initial symmetric state $|\psi_{M=2}\rangle$ with general Hamming distance d . Let $(\underbrace{|0\dots 0\rangle}_d + \underbrace{|1\dots 1\rangle}_d)\underbrace{|1\dots 1\rangle}_{n-d}$ be the two states with negative sign, then the hypergraph associated to $|\psi_{M=2}\rangle$ can be derived as follows: Group the last $n - d$ vertices with a hyperedge of order $n - d$. Then, connect the whole group to the remaining d vertices in any possible way, namely by exploiting hyperedges of any order greater than

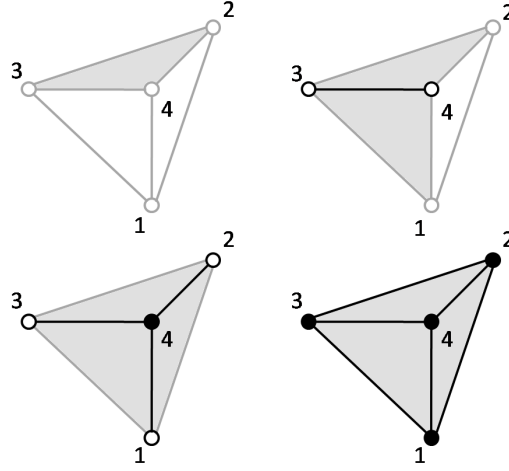


Figure 2. Hypergraphs associated to the four-qubit initial Grover states with two solutions for several values of the Hamming distance. Top-left corner: $d = 1$, top-right corner: $d = 2$, bottom-left corner: $d = 3$, and bottom-right corner: $d = 4$. Each empty vertex represents a qubit. Full dark dots, dark lines and grey faces represent hyperedges of order 1, 2 and 3, respectively. Recall that a hyperedge of order 1 represents a local Z gate. Notice that in the hypergraph with $d = 4$ also the hidden face connecting the vertices 1, 2 and 3 is present.

$n - d$ except the hyperedge of order n . The above procedure is needed because, after we have generated the desired minus signs in front the two components $|0...01...1\rangle$ and $|1...11...1\rangle$, we then have to correct the undesired by-product minuses in front of the other components that contain states $|1\rangle$ for all the last $n - d$ qubits.

Notice that both the extreme cases $d = 1$ and $d = n$ fit into this scheme. Regarding the former, since we are not allowed to draw the hyperedge of order n , we only group the last $n - 1$ vertices without connecting them to the remaining one. The biseparability of the state then follows trivially. For the latter, we do not apply the first step of the procedure above, but we connect all possible vertices according to the second step. Notice that, in order to derive the hypergraph corresponding to $|\psi_{M=2}\rangle$ with $d = n$, we have to recast $|\psi_{M=2}\rangle$ into the hypergraph state with a plus sign in front of $|0...00\rangle$, by multiplying all amplitudes by a factor -1 . As an example, the hypergraphs associated to the four-qubit symmetric states $|\psi_{M=2}\rangle$ with Hamming distance $d = 1, 2, 3$ and 4 are shown in Fig. 2.

Notice that the proposed procedure can be generalized to any initial state $|\psi_{M=2}\rangle$ by simply renaming and re-ordering the vertices.

5. Conclusions

In this paper we have explicitly computed the amount of entanglement contained in the states employed in the initial step of the Grover algorithm, namely after the first oracle call, for one and two solutions. Numerical results suggest that the entanglement content of these states, quantified by the geometric measure of entanglement, decreases

exponentially with increasing number of qubits composing the register. In the search for two items, the Hamming distance between the items is found to play a crucial role with respect to the entanglement content: For a fixed number of qubits the state turns out to be more entangled for a larger Hamming distance.

The connection with quantum hypergraph states has then been worked out, showing the mathematical hypergraphs associated to symmetric initial states with one or two solutions. We have shown that, besides giving a very convenient pictorial representation of quantum states, the hypergraph structure also highlights some entanglement properties of the states, such as biseparability or the presence of genuine multipartite entanglement.

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